

Equations of state and thermoelastic properties of the Earth's lower mantle

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Abstract The thermoelastic properties of the lower mantle of the Earth were studied using different equations of state. The values of bulk modulus and its pressure derivative, thermal expansivity, Grüneisen parameter γ and its volume derivatives, q and λ have been calculated for the entire depth of the lower mantle ranging from 670 km to 2891 km. The results obtained in the present study are found to compare well with the corresponding values based on the seismological data reported by Stacey and Davis [*Phys. Earth Planet. Inter.* **142** 137 (2004)].

Keywords Thermal expansivity, Grüneisen parameter, seismological data, bulk modulus.

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1. Introduction

The lower mantle of the Earth ranges from 670 km to 2891 km in depth and the corresponding pressure ranges 24 GPa to 136 GPa according to the Preliminary Reference Earth Model [1] (PREM), and the corresponding temperature [2] is estimated to be, for example, from 1980 K to 2940 K. Geochemical and geophysical evidences [3-5] indicate that the composition of Earth's lower mantle is primarily (Mg, Fe) SiO_3 perovskite with a little dissolved Al_2O_3 , (Mg, Fe) O magnesiowüstite, and a few percent CaSiO_3 perovskite. This composition is just simple enough to make a useful comparison of its properties with seismological data.

For understanding the thermoelastic properties of Earth's lower mantle we need equations of state (EOS) for minerals applicable at high pressures and high temperatures. The applicability of an EOS can be judged by comparing the calculated P - V results with the experimental data. However, the measured laboratory data are subject to uncertainties arising from calibration errors related to the use of pressure scales [6,7]. On the other hand, seismological data are free from calibration errors, and offer much more effective tests of high pressure equations of state than do laboratory data and can be used to recalibrate laboratory pressure scales. Geophysics offers two wide pressure ranges, one for the lower mantle and other for the core, over which there are reliable values not just of pressure, but also of bulk modulus at different densities.

In the present paper, thermoelastic properties of the lower mantle are studied using equations of state, such as, (i) Birch-Murnaghan EOS [8] (ii) Rydberg-Vinet EOS [9-11], and (iii) Shanker EOS [12]. The results are obtained for pressure P , bulk modulus K and its pressure derivative K' for the entire depth of the lower mantle, and compared with the seismological data [7] derived from the Preliminary Reference Earth model (PREM) [1] using the Stacey relationships for P , K and K' . The thermoelastic properties such as the Gruneisen parameter γ and its volume derivatives q and λ , and thermal expansivity α have been calculated and compared with the seismological data [7].

2. Method of analysis

The following three equations of state are considered

1. Birch-Murnaghan EOS:

This EOS has been derived from the Eulerian finite strain theory [8]. Expressions for pressure P , bulk modulus K and its pressure derivative $K' = dK/dP$ are given below

$$P = \frac{3}{2} K_0 (x^{-7/3} - x^{-5/3}) \left[1 + \frac{3}{4} (K'_0 - 4) (x^{-2/3} - 1) \right] \quad (1)$$

$$K = \frac{1}{2} K_0 (7x^{-7/3} - 5x^{-5/3}) + \frac{3}{8} K_0 (K'_0 - 4) (9x^{-3} - 14x^{-7/3} + 5x^{-5/3}) \quad (2)$$

$$K' = \frac{K_0}{8K} \left[(K'_0 - 4) (81x^{-3} - 98x^{-7/3} + 25x^{-5/3}) + \frac{4}{3} (49x^{-7/3} - 25x^{-5/3}) \right] \quad (3)$$

where $x = V/V_0$, K_0 and K'_0 are the values of K and K' at $P = 0$. V is the volume at pressure P and V_0 is the volume at zero pressure. Also $V/V_0 = \rho_0/\rho$ where ρ_0 is the density ρ at $P = 0$.

II. Rydberg -Vinet EOS :

Vinet *et al* [11] have obtained an EOS which is based on the potential energy function due to Rydberg [10]

$$E(r) = E(a) \left[1 - b \left(1 - \frac{r}{a} \right) \right] \exp \left[b \left(1 - \frac{r}{a} \right) \right] \quad (4)$$

Here, $E(r)$ is the potential energy expressed as a function of the interatomic distance r . For a given solid, a and b are constants. ' a ' is the equilibrium value of interatomic distance r , and ' b ' is the hardness parameter in the potential function [10]. At $r = a$, we have $E(r) = E(a)$. The EOS derived from Eq. (4) is known as the Rydberg – Vinet EOS. The expressions for P , K , and K' obtained from this EOS are given below [9,13]

$$P = 3K_0 x^{-2/3} (1 - x^{1/3}) \exp[\eta(1 - x^{1/3})] \quad (5)$$

$$K = K_0 x^{-2/3} \left[1 + \{ \eta x^{1/3} + 1 \} (1 - x^{1/3}) \right] \exp[\eta(1 - x^{1/3})] \quad (6)$$

$$K' = \frac{1}{3} \frac{x^{1/3}(1-\eta) + 2\eta x^{2/3}}{1 + (\eta x^{1/3} + 1)(1 - x^{1/3})} + \eta x^{1/3} + 2 \quad (7)$$

where $x = \frac{V}{V_0}$ and $\eta = \frac{3}{2}(K'_0 - 1)$.

III. Shanker EOS :

Shanker *et al* [12] have obtained an EOS using the volume dependence of the interatomic force constant for interatomic potentials. The force constant is defined as follows [14].

$$A = \frac{1}{3} \left(\frac{d^2 E}{dr^2} + \frac{2}{r} \frac{dE}{dr} \right) \quad (8)$$

where E is the lattice potential energy and r is the interatomic separation. The expressions based on the Shanker EOS are given below [12,15]

$$P = K_0 \frac{x^{-4/3}}{t} \left[\left(1 - \frac{1}{t} + \frac{2}{t^2} \right) \{ \exp(ty) - 1 \} + y \left(1 + y - \frac{2}{t} \right) \exp(ty) \right] \quad (9)$$

$$K = K_0 x^{-1/3} (1 + y + y^2) \exp(ty) + \frac{4}{3} P \quad (10)$$

$$K' = \frac{4}{3} + \left(1 - \frac{4}{3} \frac{P}{K} \right) \times \frac{1}{3} + x \left\{ t + \frac{(1+2y)}{(1+y+y^2)} \right\} \quad (11)$$

where $x = \frac{V}{V_0}$, $y = 1 - \left(\frac{V}{V_0}\right)$ and $t = K'_0 - \frac{8}{3}$

We make use of equations (1-3), (5-7) and (9-11) to calculate P , K and K' for the lower mantle. The Gruneisen parameter γ is an important quantity which relates thermal and elastic properties of materials. We have the following expression for γ [16]

$$\gamma = \frac{V\alpha K_T}{C_V} = \frac{V\alpha K_S}{C_P} \quad (12)$$

It is dimensionless combination of four familiar quantities, volume thermal expansion coefficient, α ; bulk modulus, K ; Volume, V ; specific heat, C ; with subscripts T , V , S , P , indicating constant temperature, volume, entropy and pressure. These alternative definitions are linked by the identities

$$\frac{K_S}{K_T} = \frac{C_P}{C_V} = 1 + \gamma\alpha T \quad (13)$$

The values of γ at different compressions can be calculated using the generalized formula for the Gruneisen parameter

$$\gamma = \frac{(1/2)K' - (1/6) - (f/3)(1 - (1/3)(P/K))}{1 - (2/3)f(P/K)} \quad (14)$$

with different values of f . The simplest of these is Slater's equation [17], for which $f = 0$. The Dugdale - MacDonald formula appears with $f = 1$, and the free - volume formula [18] with $f = 2$. Values of γ , calculated from Eq. (14) with different values of f , are not well appropriate for the lower mantle. Stacey and Davis have suggested that the general form of the free volume equation (Eq. (14)) could be used with a suitably adjusted value of f . By using the acoustic value of γ at $P = 0$, we can calculate the value of f which is $f = 1.436$ [7].

To proceed further we examine the behaviour of q and λ for the lower mantle, which are the volume derivatives of Gruneisen parameter such as

$$q = \left(\frac{\partial \ln \gamma}{\partial \ln V} \right)_T \quad (15)$$

and

$$\lambda = \left(\frac{\partial \ln q}{\partial \ln V} \right)_T \quad (16)$$

The fact that $q \rightarrow 0$ at $V \rightarrow 0$ suggested to Stacey and Isaak [19] that the next derivative

$$\lambda = \left(\frac{\partial \ln q}{\partial \ln V} \right)_T$$

might be constant, at least to a useful approximation. With constant λ , eq. (16) integrates to

$$q = q_0 \left(\frac{V}{V_0} \right)^\lambda \quad (17)$$

$$\text{and} \quad \ln \left(\frac{\gamma}{\gamma_0} \right) = \frac{q_0}{\lambda} \left(\frac{V}{V_0} \right)^\lambda - 1 \quad (18)$$

As $P \rightarrow \infty$, $V \rightarrow 0$, and $\gamma \rightarrow \gamma_\infty$, and therefore eq. (18) yields

$$\lambda = \frac{q_0}{\ln(\gamma_0/\gamma_\infty)} \quad (19)$$

However, we have no fundamental reason for believing that λ is constant, we know that it is a much better assumption than constant q , as has often been assumed in mineral physics [16,20]. In the present study, on the basis of generalized free volume theory, it is found that q as well as λ , both depend on pressure or volume. On differentiating eq. (14), we obtain the expressions for q and λ , given as follows

$$q = \frac{A_1}{A_2} \quad (20)$$

$$\lambda = \frac{A_3}{A_1 A_2} \quad (21)$$

$$\text{where} \quad A_1 = \left[-\frac{K}{2} + \frac{f}{3} P \right] K'' - \frac{2f^2}{9} \frac{P}{K} + \frac{f}{3} - \frac{f}{3} \frac{PK'}{K} K' + 2f^2 \quad (22)$$

$$A_2 = \left[\frac{K'}{2} - \frac{1}{6} - \frac{f}{3} \left\{ 1 - \frac{1}{3} \frac{P}{K} \right\} \right] 1 - \frac{2f}{3} \frac{P}{K} \quad (23)$$

and

$$\begin{aligned}
 A_3 = & \frac{K}{4} (K'K'' + KK''') \left(K' - \frac{1}{3} \right) - \frac{K^2 K'''}{4} + \frac{f}{18} \left[-9PK'^2 K'' - 6PKK'K''' - 3K^3 \right. \\
 & + \frac{3PK'''}{K} - 3K^2 K''' + 6PKK'^2 - 3KK'K'' + 6PK'K'' + 3PKK''' - 2KK'' + K'^2 \\
 & \left. \frac{PK'^3}{K} \right] + \frac{f^2}{9} \left[3K^2 - \frac{3PK'^3}{K} + 4PK'K'' + 2PKK''' + P^2 K'K''' + \frac{2P^2 K'^2 K''}{K} \right. \\
 & - P^2 K'^2 - K' + \frac{PK'^2}{K} + PK'' - P^2 K''' - \frac{3P^2 K'K''}{K} + \frac{2f^3}{81} \left[-9K' + \frac{9PK''}{K} \right. \\
 & - 3PK'' - 3P^2 K''' - \frac{9P^2 K'K''}{K} - \frac{3P^2 K'^2}{K^2} + \frac{P^3 K'''}{K} + \frac{4P^3 K'K''}{K^2} + \frac{P^3 K'^3}{K^3} + 2 \\
 & \left. \left. + \frac{4f^4}{243} \left[-\frac{3PK'}{K} + \frac{3P^2 K''}{K} + \frac{3P^2 K'}{K^2} - \frac{P^3 K'^2}{K^3} - \frac{P^3 K''}{K^2} - \frac{2P}{K} + 3 \right] \right] \right] \quad (24)
 \end{aligned}$$

where $K'' = d^2K/dP^2$ and $K''' = d^3K/dP^3$ are respectively the second and third order derivatives of bulk modulus.

The behaviour of higher derivatives is important for understanding the thermoelastic properties. However, the traditional equations of state (such as the Birch - Murnaghan EOS (1-3), the Rydberg-Vinet EOS (5-7), and the Shanker EOS (9-11)) lead to quite complicated expressions for the higher derivatives of bulk modulus (K'' and K''') and therefore less convenient to use. On the other hand, the Stacey EOS which is based on the reciprocal K -primed equation gives a slight advantage and that is in manipulating higher derivatives. Expressions for Stacey EOS are given below

$$\frac{1}{K'} = \frac{1}{K_0} + \left(1 - \frac{K'_\infty}{K_0} \right) \frac{P}{K} \quad (25)$$

where K'_∞ is the value of K' in the limit $P \rightarrow \infty$.

Eq. (25) integrates to expressions for K/K_0 and ρ/ρ_0 in terms of P/K

$$\frac{K}{K_0} = \left| 1 - K'_\infty \frac{P}{K} \right|^{-K_0/K'_\infty} \quad (26)$$

$$\ln\left(\frac{\rho}{\rho_0}\right) = -\frac{K'_0}{K_\infty^2} \ln\left(1 - K'_\infty \frac{P}{K}\right) - \left(\frac{K'_0}{K_\infty} - 1\right) \frac{P}{K} \quad (27)$$

where ρ is density of the material under study, ρ_0 is the value of ρ at $P = 0$.

By differentiating eq. (25) we can express the next two derivatives, at arbitrary compression, in terms of K' , K'_0 and K'_∞ with convenient simplicity

$$KK'' = -\frac{K'^2}{K'_0} (K' - K'_\infty) \quad (28)$$

$$\text{and} \quad K^2 K''' = \frac{K'^3}{K_0^2} (K' - K'_\infty) (3K' - 2K'_\infty + K'_0) \quad (29)$$

As $P \rightarrow \infty$, $K' \rightarrow K'_\infty$ such that

$$K'_\infty = \left(\frac{P}{K}\right)^{-1} \quad (30)$$

By fitting the data on $\rho - P - K$ for the lower mantle in the above expressions (25-29), Stacey and Davis⁷ have found $K_0 = 206\text{GPa}$, $K'_0 = 4.2$ and $K'_\infty = 2.4$. We have used these values as input in the present study.

3. Results and Discussions

First, we have calculated P , bulk modulus K and $K' = dK/dP$ as a function of density $\rho_0/\rho = V/V_0$ for the lower mantle at different values of r , the distance from the centre of Earth. Thus the range of $r(5701\text{-}3480\text{km})$ for the lower mantle corresponds to the depth $670\text{-}2891\text{km}$. We have used equations (1-3), (5-7) and (9-11) based on the Birch-Murnaghan EOS, the Rydberg-Vinet EOS and the Shanker EOS. The input data used in the present study are the zero pressure values, $K'_0 = 206\text{ GPa}$, $K'_0 = 4.2$ and $K'_\infty = 2.4$ for the lower mantle reported by Stacey and Davis [7]. The results are given in Tables 1-3. The results for pressure P , bulk modulus K and pressure derivative K' obtained from different equations are compared with the seismological data [7]. The comparison reveals that the Rydberg-Vinet EOS and the Shanker EOS yield very similar results which are close to the seismological data for the entire depth of the lower mantle. On the other hand, the Birch-Murnaghan EOS yields significant deviations.

We have also calculated thermoelastic properties such as Gruneisen parameter γ , thermal expansivity α , and volume derivatives of Gruneisen parameter q and λ for the

Table 1. Values of P(GPa) calculated from (a) Birch - Murnaghan EOS, (b) Rydberg-Vinet EOS and (c) Shanker EOS, compared with the seismological data [7] for the lower mantle

r (km)	ρ (kgm ⁻³)	$\rho_0 / \rho = V / V_0$	P(GPa) Seismological data	Calculated values of P(GPa)		
				(a)	(b)	(c)
3480	5567	0.7144	135.75	141.02	136.26	136.41
3600	5508	0.7220	128.71	133.54	129.30	129.44
3630	5493	0.7240	126.97	131.62	127.51	127.66
3800	5409	0.7353	117.35	121.24	117.80	117.94
4000	5310	0.7490	106.39	109.57	106.81	106.94
4200	5210	0.7633	95.76	98.36	96.19	96.30
4400	5108	0.7786	85.43	87.37	85.71	85.80
4600	5005	0.7946	75.36	76.88	75.64	75.71
4800	4899	0.8118	65.52	66.62	65.73	65.78
5000	4790	0.8303	55.90	56.65	56.05	56.07
5200	4677	0.8503	46.46	46.97	46.59	46.60
5400	4560	0.8721	37.29	37.57	37.35	37.35
5600	4438	0.8961	28.29	28.44	28.33	28.32
5701	4374	0.9092	23.83	23.93	23.87	23.85

Table 2. Values of K(GPa) calculated from (a) Birch - Murnaghan EOS, (b) Rydberg-Vinet EOS and (c) Shanker EOS, compared with the seismological data [7] for the lower mantle

r (km)	ρ (kgm ⁻³)	$\rho_0 / \rho = V / V_0$	K(GPa) Seismological data	Calculated values of K(GPa)		
				(a)	(b)	(c)
3480	5567	0.7144	667	721	669	670
3600	5508	0.7220	645	695	648	649
3630	5493	0.7240	640	689	643	643
3800	5409	0.7353	610	653	613	614
4000	5310	0.7490	576	613	579	580
4200	5210	0.7633	542	574	546	547
4400	5108	0.7786	509	535	512	514
4600	5005	0.7946	476	498	479	481
4800	4899	0.8118	444	461	447	448
5000	4790	0.8303	411	425	414	415
5200	4677	0.8503	379	389	382	383
5400	4560	0.8721	347	354	349	350
5600	4438	0.8961	315	320	316	317
5701	4374	0.9092	299	302	300	300

Table 3. Values of K' calculated from (a) Birch - Murnaghan EOS, (b) Rydberg-Vinet EOS and (c) Shanker EOS, compared with the seismological data [7] for the lower mantle.

r (km)	ρ (kgm ⁻³)	$\rho_0 / \rho = V / V_0$	K' Seismological data	Calculated values of K'		
				(a)	(b)	(c)
3480	5567	0.7144	3.08	3.40	3.01	2.97
3600	5508	0.7220	3.10	3.41	3.03	3.00
3630	5493	0.7240	3.10	3.41	3.04	3.00
3800	5409	0.7353	3.13	3.44	3.07	3.04
4000	5310	0.7490	3.16	3.46	3.12	3.09
4200	5210	0.7633	3.19	3.49	3.16	3.15
4400	5108	0.7786	3.23	3.53	3.21	3.21
4600	5005	0.7946	3.27	3.56	3.27	3.27
4800	4899	0.8118	3.32	3.60	3.33	3.33
5000	4790	0.8303	3.38	3.65	3.40	3.41
5200	4677	0.8503	3.45	3.70	3.47	3.49
5400	4560	0.8721	3.52	3.76	3.56	3.58
5600	4438	0.8961	3.62	3.83	3.66	3.69
5701	4374	0.9092	3.68	3.87	3.72	3.75

lower mantle at different values of r . The results for Gruneisen parameter γ and thermal expansivity α are reported in Tables 4 and 5 and compared with seismological values. The results obtained from the Rydberg-Vinet EOS and the Shanker EOS are in good agreement with the seismological values. On the other hand, the results obtained from the Birch-Murnaghan EOS are nearly ten percent higher than the seismological values. For estimating the value of q and λ , we need the higher derivatives i.e., KK'' and K^2K''' . We have calculated the values of KK'' and K^2K''' using equations (28) and (29) respectively, and then the values of q and λ with the help of equations (20)-(24). The calculated values of q and λ are reported in Table 6, and compared with the values based on seismological data [7]. It is found that the calculated values of q are in good agreement with the seismological values while the calculated values of λ are only in fair agreement with seismological values.

It should be mentioned that γ , q and λ are determined respectively from the first, second, and third pressure derivatives of bulk modulus, which are in turn related to the second, third, and fourth derivatives of pressure-volume relationships expressed in different forms of equation of state. Thus γ , q and λ can be expressed in terms of third-, fourth-, and fifth derivatives of potential energy function respectively. The calculation of λ is therefore most sensitive to the form of the potential function or the equation of state used as it depends on the third pressure derivative of bulk modulus.

Table 4. Values of γ calculated from modified free volume formula [eq. (14)] with $f = 1.436$ using different EOS (a) Birch-Murnaghan EOS, (b) Rydberg-Vinet EOS, (c) Shanker EOS and (d) Seismological data [7].

r (km)	(a)	(b)	(c)	(d) Seismological data
3480	1.3360	1.1082	1.0832	1.1412
3600	1.3359	1.1142	1.0957	1.1447
3630	1.3340	1.1186	1.0942	1.1454
3800	1.3430	1.1278	1.1092	1.1515
4000	1.3428	1.1465	1.1282	1.1591
4200	1.3482	1.1581	1.1519	1.1676
4400	1.3579	1.1745	1.1738	1.1757
4600	1.3603	1.1955	1.1947	1.1881
4800	1.3667	1.2140	1.2136	1.2008
5000	1.3765	1.2365	1.2417	1.2154
5200	1.3839	1.2557	1.2667	1.2335
5400	1.3930	1.2831	1.2938	1.2548
5600	1.4032	1.3115	1.3273	1.2815
5701	1.4090	1.3285	1.3446	1.2972

Table 5. Values of thermal expansivity α (10^{-6}K^{-1}) from eq. (12) corresponding to the results for γ given in Table 4.

r (km)	(a)	(b)	(c)	(d) Seismological data
3480	12.6	11.0	10.8	11.3
3600	12.7	11.2	11.0	11.6
3630	12.8	11.3	11.1	11.7
3800	13.4	11.8	11.6	12.1
4000	14.0	12.5	12.3	12.7
4200	14.7	13.1	13.0	13.4
4400	15.6	14.0	13.9	14.2
4600	16.5	14.9	14.8	15.0
4800	17.6	15.9	15.9	15.9
5000	18.8	17.2	17.2	17.0
5200	20.2	18.5	18.6	18.3
5400	21.8	20.2	20.4	19.8
5600	23.8	22.3	22.5	21.8
5701	25.0	23.5	23.8	23.0

Table 6. Values of q and λ ; (a) calculated from eq. (20) and eq. (21) with $f = 1.436$, and comparison with (b) the values based on seismological data [7].

r (km)	q (a)	λ (a)	q (b)	λ (b)
3480	0.3058	3.72	0.2770	3.36
3600	0.3176	3.91	0.2894	3.37
3630	0.3196	3.77	0.2926	3.37
3800	0.3395	4.01	0.3117	3.39
4000	0.3641	4.01	0.3365	3.41
4200	0.3935	3.90	0.3644	3.43
4400	0.4252	4.05	0.3919	3.45
4600	0.4634	4.03	0.4324	3.50
4800	0.5064	4.19	0.4748	3.54
5000	0.5453	4.69	0.5245	3.60
5200	0.6187	4.78	0.5860	3.67
5400	0.7013	4.71	0.6602	3.76
5600	0.7992	5.11	0.7549	3.88
5701	0.8592	5.37	0.8136	3.94

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References

- [1] A M Dziewonski and D L Anderson *Phys. Earth Planet Inter.* **25** 297 (1981)
- [2] D L Anderson and R Philas *Trans. Soc. London Ser. A* **306** 21 (1982)
- [3] E Ito and E Takahashi *Geophys. Monograph* **39** 221 (1987)
- [4] D L Anderson *Theory of the Earth* (Boston : Blackwell Scientific Publications)
- [5] C R Bina *Phys. Chem. of the Earth's Deep Inter.* **37** 205 (1998)
- [6] F D Stacey *Phys. Earth Planet Inter.* **128** 179 (2001)
- [7] F D Stacey and P M Davis *Phys. Earth Planet Inter.* **142** 137 (2004)
- [8] F Birch *J. Geophys Res.* **57** 227 (1952)
- [9] F D Stacey, B J Brennan and R D Irvine *Geophys. Surveys* **4** 189 (1981)
- [10] R Rydberg *Z. Phys.* **73** 376 (1932)
- [11] P Vinet, J H Rose, J Ferrante and J R Smith *J. Phys. Condens. Matter* **1** 1941 (1989)
- [12] J Shanker, S S Kushwah and P Kumar *Physica B* **239** 337 (1997)
- [13] S Gaurav, B S Sharma, S B Sharma and S C Upadhyaya *Physica B* **322** 328 (2002)
- [14] M Born, and K Huang, *Dynamical Theory of Crystal Lattices*, (Oxford : Clarendon Press) p110 (1954)

- [15] J Shanker and S S Kushwah and M P Sharma *Physica B* **271** 158 (1999)
- [16] O L Anderson *Equations of state of solids for geophysics and ceramic science* (New York Oxford University Press) (1995)
- [17] J C Slater *Introduction of Chemical Physics* (New York : Mc Graw-Hill) 521 (1939)
- [18] V Vashchenko and V N Zubarev *Sov. Phys. Solid State* **5** 653 (1963)
- [19] F D Stacey and D G Isaak *Geophys. J. Int.* **146** 143 (2001)
- [20] R Jeanloz *J. Geophys. Res.* **94** 5873 (1989)